29 March 1996

ELSEVIER

Chemical Physics Letters 251 (1996) 416–422

CHEMICAL PHYSICS LETTERS

Author index to volume 251

Aiga, F. and R. Itoh, Calculation of frequency-dependent polarizabilities and hyperpolarizabilities by the second-order Møller–Plesset perturbation theory 251 (1996) 372
Alasia, F., see Roman, H.E. 251 (1996) 111
Amos, R.D., see Ioannou, A.G. 251 (1996) 52
Aratono, Y., see Kumada, T. 251 (1996) 219
Arnaud, R., see Barone, V. 251 (1996) 393

Bagus, P.S., H.J. Freund, T. Minerva, G. Pacchioni and F. Parmigiani, Charge transfer effects and photoemission in transition metal oxides 251 (1996) 90
Baldwin, M., see Heller, J. 251 (1996) 223
Barone, V. and R. Arnaud, Study of prototypical Diels–Alder reactions by a hybrid density functional/Hartree–Fock approach 251 (1996) 393
Baxter, G.W., M.J. Johnson, J.G. Haub and B.J. Orr, OPO CARS: coherent anti-Stokes Raman spectroscopy using tunable optical parametric oscillators injection-seeded by external-cavity diode lasers 251 (1996) 211
Belchior, J.C., J.R. Pliego Jr. and J.P. Braga, A comparison of state-to-state rotational total cross sections using two- and three-dimensional close coupled approaches 251 (1996) 346
Bemish, R.J., M.C. Chan and R.E. Miller, Molecular control using dc electric fields: quenching of the tunneling in HF dimer 251 (1996) 182
Bennati, M., see Surján, P.R. 251 (1996) 115
Bennett, F.R. and I.R. McNab, The infrared spectrum of HCl^{2+} and its isotopomers 251 (1996) 405
Bernhardsson, A., R. Lindh, G. Karlström and B.O. Roos, Direct self-consistent reaction field with Pauli repulsion: solvation effects on methylene peroxide 251 (1996) 141
Bisht, P.B., G.C. Joshi and H.B. Tripathi, Excited state hydrogen bonding of the 2-naphthol–triethylamine system in 1,4-dioxane (Chem. Phys. Letters 237 (1995) 356). Erratum 251 (1996) 413
Bloemink, H.I., C.M. Evans, J.H. Holloway and A.C. Legon, Are B · · · Cl–F bonds linear? The angular geometry of a pre-reactive complex of oxirane and chlorine monofluoride from rotational spectroscopy 251 (1996) 275
Boguslavsky, A.A., see Semin, G.K. 251 (1996) 250
Bonham, R.A., see Mi, L. 251 (1996) 252
Borg, R.A.J., see Waclawik, E.R. 251 (1996) 95
Bosi, L., D. Gallo and M. Zelada, The NaCl : Cu^{+} de-excitation mechanism revisited 251 (1996) 335
Bovensmann, H., see Himmelmann, S. 251 (1996) 330
Braga, J.P., see Belchior, J.C. 251 (1996) 346
Bratu, P., K.L. Kompa and U. Höfer, Optical second-harmonic investigations of H_2 and D_2 adsorption on Si(100)2 × 1: the surface temperature dependence of the sticking coefficient 251 (1996) 1

Broglia, R.A., see Roman, H.E. 251 (1996) 111
Burrows, J.P., see Himmelmann, S. 251 (1996) 330

Cadioli, B., see Fowler, P.W. 251 (1996) 132
Caminati, W., G. Maccaferri, P.G. Favero and L.B. Favero, Free jet absorption millimeter wave spectrum of purine 251 (1996) 189
Cederbaum, L.S., see Handke, G. 251 (1996) 26
Chan, M.C., see Bemish, R.J. 251 (1996) 182
Chen, W.Z., see Wang, C.X. 251 (1996) 268
Clougherty, D.P. and J.P. Gorman, On the vibrational modes of C_{60} 251 (1996) 353
Collings, B.A., see McComb, D.W. 251 (1996) 8
Colò, G., see Roman, H.E. 251 (1996) 111
Cotterell, B.J., see Stickland, R.J. 251 (1996) 287

Daehne, S., see De Rossi, U. 251 (1996) 259
De Rossi, U., S. Daehne and R. Reisfeld, Photophysical properties of cyanine dyes in sol–gel matrices 251 (1996) 259
De Silvestri, S., see Lanzani, G. 251 (1996) 339
Dong, R.Y., On the detection of second-order director fluctuations at a standard high field by spin–spin relaxation 251 (1996) 387
Douillard, R., see Wang, C.X. 251 (1996) 268
Dressler, R.A., see Levandier, D.J. 251 (1996) 174

Eilers, H. and B.M. Tissue, Laser spectroscopy of nanocrystalline Eu_2O_3 and Eu^{3+}:Y_2O_3 251 (1996) 74
Ernst, M., see Heller, J. 251 (1996) 223
Evans, C.M., see Bloemink, H.I. 251 (1996) 275

Favero, L.B., see Caminati, W. 251 (1996) 189
Favero, P.G., see Caminati, W. 251 (1996) 189
Fowler, P.W., R. Zanasi, B. Cadioli and E. Steiner, Ring currents and magnetic properties of pyracylene 251 (1996) 132
Francisco, J.S., see Lee, T.J. 251 (1996) 400
Freed, J.H., see Saxena, S. 251 (1996) 102
Freund, H.J., see Bagus, P.S. 251 (1996) 90
Friend, R.H., see Grüner, J. 251 (1996) 204
Fujii, T.S. and S. Iwata, Theoretical studies of the ground and low-lying excited electronic states of the early transition metal dihydrides with state averaged MC SCF method 251 (1996) 150

Gallo, D., see Bosi, L. 251 (1996) 335
Gascooke, J.R., see Waclawik, E.R. 251 (1996) 95
Geerlings, P., see Verbandt, Y. 251 (1996) 47
Goldman, S., see Joslin, C.G. 251 (1996) 414
Gorman, J.P., see Clougherty, D.P. 251 (1996) 353
Gray, C.G., see Joslin, C.G. 251 (1996) 414
Gropen, O., see Heß, B.A. 251 (1996) 365
Grüner, J., R.H. Friend, J. Huber and U. Scherf, A blue-luminescent ladder-type poly(para-phenylene) copolymer containing oxadiazole groups 251 (1996) 204
Grupp, A., see Surján, P.R. 251 (1996) 115

Güdel, H.U., see Hazenkamp, M.F. 251 (1996) 301
Güthe, F., see Weitzel, K.-M. 251 (1996) 295

Hackett, P.A., see McComb, D.W. 251 (1996) 8
Handke, G., F. Tarantelli and L.S. Cederbaum, On the calculation of shake-off satellite contributions to molecular Auger spectra 251 (1996) 26
Handy, N.C., see Ioannou, A.G. 251 (1996) 52
Haub, J.G., see Baxter, G.W. 251 (1996) 211
Hazenkamp, M.F. and H.U. Güdel, Near-infrared luminescence of chromium(V)-doped Li_3PO_4 251 (1996) 301
Heller, J., R. Larsen, M. Ernst, A.C. Kolbert, M. Baldwin, S.B. Prusiner, D.E. Wemmer and A. Pines, Application of rotational resonance to inhomogeneously broadened systems 251 (1996) 223
Heß, B.A., C.M. Marian, U. Wahlgren and O. Gropen, A mean-field spin–orbit method applicable to correlated wavefunctions 251 (1996) 365
Hickman, C.G., see Waclawik, E.R. 251 (1996) 95
Himmelmann, S., J. Orphal, H. Bovensmann, A. Richter, A. Ladstätter-Weissenmayer and J.P. Burrows, First observation of the OIO molecule by time-resolved flash photolysis absorption spectroscopy 251 (1996) 330
Höfer, U., see Bratu, P. 251 (1996) 1
Holloway, J.H., see Bloemink, H.I. 251 (1996) 275
Hrbek, J., see Rodriguez, J.A. 251 (1996) 13
Huber, J., see Grüner, J. 251 (1996) 204
Hulse, J.E., see McComb, D.W. 251 (1996) 8
Hupp, J.T., see Yoon, D.I. 251 (1996) 84
Hurley, M.D., see Wallington, T.J. 251 (1996) 164

Inagaki, H., see Kumada, T. 251 (1996) 219
Ioannou, A.G., R.D. Amos and N.C. Handy, The diagonal Born–Oppenheimer correction for He_2^+ and $F + H_2$ 251 (1996) 52
Itoh, R., see Aiga, F. 251 (1996) 372
Iwata, S., see Fujii, T.S. 251 (1996) 150

Johnson, M.J., see Baxter, G.W. 251 (1996) 211
Joshi, G.C., see Bisht, P.B. 251 (1996) 413
Joslin, C.G., C.G. Gray and S. Goldman, Infrared rotation and vibration–rotation bands of endohedral fullerene complexes. He@C_{70} (Chem. Phys. Letters 244 (1995) 93). Erratum 251 (1996) 414

Kambe, N., see Sugino, T. 251 (1996) 125
Karlström, G., see Bernhardsson, A. 251 (1996) 141
Käß, H. and W. Lubitz, Evaluation of 2D-ESEEM data of ^{15}N-labeled radical cations of the primary donor P_{700} in photosystem I and chlorophyll **a** 251 (1996) 193
Kawasaki, M., Y. Sato, K. Suto, Y. Matsumi and S.H.S. Wilson, Ion imaging of the photodissociation of HNCO near 217 nm 251 (1996) 67
Kettunen, P., see Steinbock, O. 251 (1996) 305
Kierzkowski, P., B. Pranszke, P. Woliński and A. Kowalski, Electronic branching ratios in the chemiluminescent reactions of Ca(^1S) and Ca*(^3P) with ICl and IBr 251 (1996) 323
Kolbert, A.C., see Heller, J. 251 (1996) 223

Kompa, K.L., see Bratu, P. 251 (1996) 1
Kowalski, A., see Kierzkowski, P. 251 (1996) 323
Kuhn, M., see Rodriguez, J.A. 251 (1996) 13
Kulkarni, G.U., see Sankar, G. 251 (1996) 79
Kumada, T., H. Inagaki, T. Nagasawa, Y. Aratono and T. Miyazaki, Experimental observation of H_2^- anions by high-resolution ESR spectroscopy in γ-ray irradiated quantum solid parahydrogen at 4.2 K 251 (1996) 219

Ladstätter-Weissenmayer, A., see Himmelmann, S. 251 (1996) 330
Lanzani, G., M. Nisoli, S. De Silvestri and R. Tubino, Femtosecond vibrational and torsional energy redistribution in photoexcited oligothiophenes 251 (1996) 339
Larsen, R., see Heller, J. 251 (1996) 223
Latanowicz, L., see Reynhardt, E.C. 251 (1996) 235
Lawrance, W.D., see Waclawik, E.R. 251 (1996) 95
Lee, T.J. and J.S. Francisco, The proton affinity of HOBr 251 (1996) 400
Legon, A.C., see Bloemink, H.I. 251 (1996) 275
Levandier, D.J., R.A. Dressler and E. Murad, A study of isotope effects in the reaction $O^+ + H_2O/D_2O \rightarrow OH^+/OD^+ + OH/OD$ using guided-ion beams 251 (1996) 174
Lindh, R., see Bernhardsson, A. 251 (1996) 141
Liu, H.-J., see Yoon, D.I. 251 (1996) 84
Lu, H., see Yoon, D.I. 251 (1996) 84
Lubitz, W., see Käß, H. 251 (1996) 193

Maccaferri, G., see Caminati, W. 251 (1996) 189
MacPherson, C.D., see McComb, D.W. 251 (1996) 8
Makarov, D.E. and M. Topaler, On the transition from electronically nonadiabatic to solvent-controlled electron transfer (Chem. Phys. Letters 245 (1995) 343). Erratum 251 (1996) 415
Malkin, S., see Puchenkov, O.V. 251 (1996) 242
Marian, C.M. and U. Wahlgren, A new mean-field and ECP-based spin–orbit method. Applications to Pt and PtH 251 (1996) 357
Marian, C.M., see Heß, B.A. 251 (1996) 365
Matsumi, Y., see Kawasaki, M. 251 (1996) 67
McComb, D.W., B.A. Collings, R.A. Wolkow, D.J. Moffatt, C.D. MacPherson, D.M. Rayner, P.A. Hackett and J.E. Hulse, An atom-resolved view of silicon nanoclusters 251 (1996) 8
McNab, I.R., see Bennett, F.R. 251 (1996) 405
Mehring, M., see Surján, P.R. 251 (1996) 115
Mi, L., C.R. Sporleder and R.A. Bonham, Covariance matrix mass spectral maps of polar dissociation channels in CF_4 251 (1996) 252
Miller, R.E., see Bemish, R.J. 251 (1996) 182
Minerva, T., see Bagus, P.S. 251 (1996) 90
Miyazaki, T., see Kumada, T. 251 (1996) 219
Moffatt, D.J., see McComb, D.W. 251 (1996) 8
Mottley, C., see Yoon, D.I. 251 (1996) 84
Mudjijono, , see Waclawik, E.R. 251 (1996) 95
Murad, E., see Levandier, D.J. 251 (1996) 174

Nagasawa, T., see Kumada, T. 251 (1996) 219
Nagata, T., see Tsukuda, T. 251 (1996) 309

Nakano, M., S. Yamada, I. Shigemoto and K. Yamaguchi, Theoretical study on the geometry dependence of the second hyperpolarizability of the allyl cation based on a numerical Liouville three-type analysis 251 (1996) 381
Németh, K., see Surján, P.R. 251 (1996) 115
Nisoli, M., see Lanzani, G. 251 (1996) 339
Novoa, J.J., M. Planas and M.C. Rovira, On the usefulness of the counterpoise method on hydrogen-bonded complexes: a numerical test using near complete basis sets on $H_2O \ldots HF$, $(H_2O)_2$, $(HF)_2$ and $CH_4 \ldots H_2O$ 251 (1996) 33

Ohta, K., see Sugino, T. 251 (1996) 125
Orphal, J., see Himmelmann, S. 251 (1996) 330
Orr, B.J., see Baxter, G.W. 251 (1996) 211

Pacchioni, G., see Bagus, P.S. 251 (1996) 90
Parmigiani, F., see Bagus, P.S. 251 (1996) 90
Pines, A., see Heller, J. 251 (1996) 223
Planas, M., see Novoa, J.J. 251 (1996) 33
Pliego Jr., J.R., see Belchior, J.C. 251 (1996) 346
Poborchii, V.V., Polarized Raman and optical absorption spectra of the mordenite single crystals containing sulfur, selenium, or tellurium in the one-dimensional nanochannels 251 (1996) 230
Pranszke, B., see Kierzkowski, P. 251 (1996) 323
Prusiner, S.B., see Heller, J. 251 (1996) 223
Puchenkov, O.V. and S. Malkin, On the time resolution of picosecond phase grating spectroscopy in tracing structural relaxation dynamics 251 (1996) 242

Rao, C.N.R., see Sankar, G. 251 (1996) 79
Ratner, M.A., see Yoon, D.I. 251 (1996) 84
Rayner, D.M., see McComb, D.W. 251 (1996) 8
Reisfeld, R., see De Rossi, U. 251 (1996) 259
Reynhardt, E.C. and L. Latanowicz, Molecular motions in solid saccharides studied by NMR spectroscopy 251 (1996) 235
Richter, A., see Himmelmann, S. 251 (1996) 330
Rodriguez, J.A., M. Kuhn and J. Hrbek, The bonding of sulfur to a Pt(111) surface: photoemission and molecular orbital studies 251 (1996) 13
Roman, H.E., G. Colò, F. Alasia and R.A. Broglia, Long wavelength optical response of incipient fullerene nanotubes 251 (1996) 111
Roos, B.O., see Bernhardsson, A. 251 (1996) 141
Rovira, M.C., see Novoa, J.J. 251 (1996) 33

Saeki, M., see Tsukuda, T. 251 (1996) 309
Sakaguchi, T., see Sugino, T. 251 (1996) 125
Samulski, E.T., see Terzis, A.F. 251 (1996) 157
Sankar, G., J.M. Thomas, V. Varma, G.U. Kulkarni and C.N.R. Rao, An investigation of the first-order spin-state transition in $Fe(Phen)_2(NCS)_2$ EXAFS and infrared spectroscopy 251 (1996) 79
Sato, Y., see Kawasaki, M. 251 (1996) 67
Saxena, S. and J.H. Freed, Double quantum two-dimensional Fourier transform electron spin resonance: distance measurements 251 (1996) 102

Scherf, U., see Grüner, J. 251 (1996) 204
Schneider, W.F., see Wallington, T.J. 251 (1996) 164
Selmarten, D.C., see Yoon, D.I. 251 (1996) 84
Semin, G.K. and A.A. Boguslavsky, NQR determination of local magnetic fields in senarmonite (Sb_2O_3) 251 (1996) 250
Shigemoto, I., see Nakano, M. 251 (1996) 381
Sonoda, N., see Sugino, T. 251 (1996) 125
Sporleder, C.R., see Mi, L. 251 (1996) 252
Steinbock, O. and P. Kettunen, Chemical clocks on the basis of rotating waves. Measuring irrational numbers from period ratios 251 (1996) 305
Steiner, E., see Fowler, P.W. 251 (1996) 132
Stickel, R.E., see Zhao, Z. 251 (1996) 59
Stickland, R.J. and B.J. Cotterell, Infrared inter-Rydberg emission spectra as a possible probe of molecular hydrogen in astrophysical environments 251 (1996) 287
Sugino, T., N. Kambe, N. Sonoda, T. Sakaguchi and K. Ohta, Ab initio molecular orbital calculations of the static polarizabilities of xanthone analogues 251 (1996) 125
Surján, P.R., K. Németh, M. Bennati, A. Grupp and M. Mehring, Zero-field-splitting in the lowest triplet state of C_{60} 251 (1996) 115
Suto, K., see Kawasaki, M. 251 (1996) 67

Tarantelli, F., see Handke, G. 251 (1996) 26
Terzis, A.F. and E.T. Samulski, Spatial distribution functions: liquid CH_3CN and CO_2 251 (1996) 157
Thienpont, H., see Verbandt, Y. 251 (1996) 47
Thomas, J.M., see Sankar, G. 251 (1996) 79
Tissue, B.M., see Eilers, H. 251 (1996) 74
Topaler, M., see Makarov, D.E. 251 (1996) 415
Tran, V., see Wang, C.X. 251 (1996) 268
Tripathi, H.B., see Bisht, P.B. 251 (1996) 413
Tsukuda, T., M. Saeki and T. Nagata, Formation of $[(CO_2)_nCH_3I]^-$ anions in the reaction of $(CO_2)_N^-$ with CH_3I 251 (1996) 309
Tubino, R., see Lanzani, G. 251 (1996) 339

Van Zant, L.C., see Watts, J.D. 251 (1996) 119
Varma, V., see Sankar, G. 251 (1996) 79
Verbandt, Y., H. Thienpont, I. Veretennicoff and P. Geerlings, Optical properties of pyrrole oligomers: a coupled quantum oscillator approach 251 (1996) 47
Veretennicoff, I., see Verbandt, Y. 251 (1996) 47

Waclawik, E.R., R.A.J. Borg, Mudjijono, J.R. Gascooke, C.G. Hickman and W.D. Lawrance, An investigation of vibration to rotation transfer in vibrational relaxation of S_1 aromatics 251 (1996) 95
Wahlgren, U., see Heß, B.A. 251 (1996) 365
Wahlgren, U., see Marian, C.M. 251 (1996) 357
Wallington, T.J., M.D. Hurley and W.F. Schneider, Atmospheric chemistry of CH_3Cl: mechanistic study of the reaction of CH_2ClO_2 radicals with HO_2 251 (1996) 164
Wang, C.X., W.Z. Chen, V. Tran and R. Douillard, Analysis of interfacial water structure and dynamics in α-maltose solution by molecular dynamics simulation 251 (1996) 268
Watts, J.D. and L.C. Van Zant, On the structure of HBPH 251 (1996) 119

Weitzel, K.-M. and F. Güthe, The distinction of direct and pulsed-field ionized zero kinetic energy photoelectrons in electron/ion coincidence experiments 251 (1996) 295
Wemmer, D.E., see Heller, J. 251 (1996) 223
Werst, D.W., Self-exchange reactions of radical anions in n-hexane 251 (1996) 315
Whitten, J.L., see Yang, H. 251 (1996) 20
Wilson, S.H.S., see Kawasaki, M. 251 (1996) 67
Wine, P.H., see Zhao, Z. 251 (1996) 59
Woliński, P., see Kierzkowski, P. 251 (1996) 323
Wolkow, R.A., see McComb, D.W. 251 (1996) 8

Yamada, S., see Nakano, M. 251 (1996) 381
Yamaguchi, K., see Nakano, M. 251 (1996) 381
Yang, H. and J.L. Whitten, Chemisorption of CNH_2 and HCNH on the Ni(111) surface 251 (1996) 20
Yoon, D.I., D.C. Selmarten, H. Lu, H.-J. Liu, C. Mottley, M.A. Ratner and J.T. Hupp, Spectroscopic and photophysical studies of apparent cluster-to-organic-acceptor charge transfer in a molecular cadmium sulfide assembly 251 (1996) 84

Zanasi, R., see Fowler, P.W. 251 (1996) 132
Zelada, M., see Bosi, L. 251 (1996) 335
Zhao, Z., R.E. Stickel and P.H. Wine, Branching ratios for methyl elimination in the reactions of OD radicals and Cl atoms with CH_3SCH_3 251 (1996) 59